

Quantum phases of dipolar spinor condensates

S. Yi¹, L. You², and H. Pu¹

¹*Department of Physics and Astronomy, and Rice Quantum Institute,
Rice University, Houston, TX 77251-1892, USA*

²*School of Physics, Georgia Institute of Technology, Atlanta, GA 30332-0430, USA*

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We study the zero-temperature ground state structure of a spin-1 condensate with magnetic dipole-dipole interactions. We show that the dipolar interactions break the rotational symmetry of the Hamiltonian and induce new quantum phases. Different phases can be reached by tuning the effective strength of the dipolar interactions via modifying the trapping geometry. The experimental feasibility of detecting these phases is investigated. The spin-mixing dynamics is also studied.

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A dipolar condensate is a condensate possessing the dipole-dipole interactions, in addition to the usual *s*-wave contact interaction. Recent theoretical studies have found that, the long-range dipolar interactions (which may originate either from the intrinsic atomic [1] or molecular [2, 3, 4] magnetic dipole moments or from the induced electric dipole moments [5]) may greatly affect the stability of the condensate [5, 6, 7, 8] and significantly modify the excitation spectrum [9, 10, 11, 12]. Furthermore, the dipolar interactions are responsible for the generation of translational entanglement [13] and a variety of novel quantum phases [14] in condensates confined in optical lattices. All these works have focused on scalar condensates. The effect of the dipolar interactions on spinor condensates confined in multi-well potentials is explored in the works of Refs. [15], where only the the dipolar interactions between different potential wells are taken into account. In this Letter, we study the properties of dipolar spinor condensates in a single trap. We show that the interplay between the spin-exchange and the dipolar interactions gives rise to extremely rich physics unexplored so far and that as the effective dipolar strength depends on the condensate aspect ratio, transitions between new quantum phases resulting from the dipolar interactions can be induced by modifying the trap geometry.

The intrinsic magnetic dipole moment of an atom is related to its total angular momentum as $\mu_F = -g_F\mu_B\mathbf{F}$, with g_F being the Landé *g*-factor, μ_B the Bohr magneton, and \mathbf{F} the angular momentum operator. Thus the dipole-dipole interactions will affect the condensate once the spin degrees of freedom become accessible as in an optical trap. Since the first creation of spinor condensates in dilute alkali atomic vapors [16], we have witnessed tremendous experimental and theoretical studies on these systems [17, 18, 19, 20, 21, 22, 23, 24]. The key feature of the spinor condensate is the spin-exchange interaction which is responsible for a variety of interesting physics such as the spin-mixing [21], phase conjugation [23], spin domain formation [16] and topological defects generation [24]. All these studies, however, neglected the dipolar interactions, except in Ref. [25], where Gu suggested that the internal dipolar field may induce spontaneous magnetization in a spinor condensate. Neverthe-

less, the dipolar interactions are not treated explicitly in that work.

Consider a spin-1 condensate with N atoms. The Hamiltonian without the dipolar intereactions, in second quantized form, reads [20]

$$H_{\text{sp}} = \int d\mathbf{r} \hat{\psi}_\alpha^\dagger(\mathbf{r}) \left(-\frac{\hbar^2 \nabla^2}{2M} + V_{\text{ext}} \right) \hat{\psi}_\alpha(\mathbf{r}) + \frac{c_0}{2} \int d\mathbf{r} \hat{\psi}_\alpha^\dagger(\mathbf{r}) \hat{\psi}_\beta^\dagger(\mathbf{r}) \hat{\psi}_\alpha(\mathbf{r}) \hat{\psi}_\beta(\mathbf{r}) + \frac{c_2}{2} \int d\mathbf{r} \hat{\psi}_\alpha^\dagger(\mathbf{r}) \hat{\psi}_{\alpha'}^\dagger(\mathbf{r}) \mathbf{F}_{\alpha\beta} \cdot \mathbf{F}_{\alpha'\beta'} \hat{\psi}_\beta(\mathbf{r}) \hat{\psi}_{\beta'}(\mathbf{r}),$$

where M is the mass of the atom, $\hat{\psi}_\alpha(\mathbf{r})$ ($\alpha = 0, \pm 1$) denotes the annihilation operator for the $m_F = \alpha$ component of a spin-1 field. The trapping potential V_{ext} is assumed to be spin-independent. The collisional interaction parameters are $c_0 = 4\pi\hbar^2(a_0 + 2a_2)/(3M)$ and $c_2 = 4\pi\hbar^2(a_2 - a_0)/(3M)$ with a_f ($f = 0, 2$) being the *s*-wave scattering length for spin-1 atoms in the combined symmetric channel of total spin f . For the two experimentally realized spinor condensate systems (²³Na and ⁸⁷Rb), we have $|c_2| \ll c_0$.

The Hamiltonian for the dipolar interactions reads

$$H_{\text{dd}} = \frac{c_d}{2} \int d\mathbf{r} \int d\mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|^3} \times \left[\hat{\psi}_\alpha^\dagger(\mathbf{r}) \hat{\psi}_{\alpha'}^\dagger(\mathbf{r}') \mathbf{F}_{\alpha\beta} \cdot \mathbf{F}_{\alpha'\beta'} \hat{\psi}_\beta(\mathbf{r}) \hat{\psi}_{\beta'}(\mathbf{r}') - 3 \hat{\psi}_\alpha^\dagger(\mathbf{r}) \hat{\psi}_{\alpha'}^\dagger(\mathbf{r}') \mathbf{F}_{\alpha\beta} \cdot \mathbf{e} \hat{\psi}_\beta(\mathbf{r}) \hat{\psi}_{\beta'}(\mathbf{r}') \right],$$

where $c_d = \mu_0 \mu_B^2 g_F^2 / (4\pi)$ and $\mathbf{e} = (\mathbf{r} - \mathbf{r}') / |\mathbf{r} - \mathbf{r}'|$ is a unit vector. The total Hamiltonian is then $H_{\text{tot}} = H_{\text{sp}} + H_{\text{dd}}$, from which we can derive the Hesenberg equations for the boson field operators. In the standard mean-field treatment, one replaces the field operators $\hat{\psi}_\alpha$ by their expectation values $\phi_\alpha \equiv \langle \hat{\psi}_\alpha \rangle$, which yields the so-called Gross-Pitaevskii equations (GPEs).

Before proceeding further, let us first estimate the relative strengths of the spin-exchange and the dipolar interactions which are characterized by c_2 and c_d , respectively. If we take $a_0 = 50a_B$ (a_B being the Bohr radius)

and $a_2 = 55a_B$ for ^{23}Na [22], we find $c_d/|c_2| \simeq 0.007$. Similarly, for ^{87}Rb ($a_0 = 101.8a_B$ and $a_2 = 100.4a_B$ [22]), we have $c_d/|c_2| \simeq 0.1$. Hence at least for ^{87}Rb , the dipolar interaction is not negligible compared to the spin-exchange interaction.

The facts that $|c_2| \ll c_0$ and $c_d \ll |c_2|$ inspire us to invoke the single mode approximation (SMA) [21], namely, $\hat{\psi}_\alpha(\mathbf{r}) \approx \phi(\mathbf{r})\hat{a}_\alpha$, where $\phi(\mathbf{r})$ is the *spin-independent* condensate spatial wave function, \hat{a}_α is the annihilation operator for $m_F = \alpha$ component. The validity of the SMA can be checked by solving the GPEs numerically for the ground state wave functions ϕ_α . We have performed these calculations and found that the SMA is valid for $c_d \lesssim 0.2|c_2|$ with scattering lengths of ^{23}Na and ^{87}Rb .

The Hamiltonian H_{sp} under the SMA is given by (after dropping spin-independent constant terms) [21]:

$$H_{\text{sp}} = c'_2 \hat{\mathbf{L}}^2, \quad (1)$$

where $c'_2 = (c_2/2) \int d\mathbf{r} |\phi(\mathbf{r})|^4$ is the spin-exchange interaction coefficient, and $\hat{\mathbf{L}} = \hat{a}_\alpha^\dagger \mathbf{F}_{\alpha\beta} \hat{a}_\beta$ is the total many-body angular momentum operator of the system, whose eigenstates and eigenvalues are defined by

$$\hat{\mathbf{L}}^2 |l, m\rangle = l(l+1) |l, m\rangle, \quad \hat{L}_z |l, m\rangle = m |l, m\rangle,$$

where $m = 0, \pm 1, \dots, \pm l$ and for a given total number of atoms N , the allowable values of l are $l = 0, 2, 4, \dots, N$ for even N and $l = 1, 3, 5, \dots, N$ for odd N . The ground state properties of the spinor condensate under H_{sp} is therefore completely determined by the sign of c'_2 [21]: For $c'_2 > 0$ (antiferromagnetic), the ground state is given by the spin singlet $|G\rangle = |0, 0\rangle$; for $c'_2 < 0$ (ferromagnetic), it is given by $|G\rangle = |N, m\rangle$ which has a $(2N+1)$ -fold degeneracy with m taking any integer numbers between $-N$ and N .

The dipolar interaction Hamiltonian under the SMA is given by

$$H_{\text{dd}} = \frac{c_d}{2} \int d\mathbf{r} \int d\mathbf{r}' \frac{|\phi(\mathbf{r})|^2 |\phi(\mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|^3} \left[(\hat{\mathbf{L}}^2 - 3(\hat{\mathbf{L}} \cdot \mathbf{e})^2) - (2N - 3\hat{a}_\alpha^\dagger \mathbf{F}_{\alpha\beta} \cdot \mathbf{e} \mathbf{F}_{\beta\beta'} \cdot \mathbf{e} \hat{a}_{\beta'}) \right]. \quad (2)$$

In general, this is still in a very complicated form. Remarkably, for a condensate with axial symmetry (which happens to be the most experimentally relevant case), with its symmetry axis chosen to be along the quantization axis, z , H_{dd} takes a very simple form:

$$H_{\text{dd}} = -c'_d \hat{\mathbf{L}}^2 + 3c'_d (\hat{L}_z^2 + \hat{n}_0), \quad (3)$$

where $\hat{n}_0 = \hat{a}_0^\dagger \hat{a}_0$ is the number operator for $m_F = 0$ and $c'_d = (c_d/4) \int \int d\mathbf{r} d\mathbf{r}' |\phi(\mathbf{r})|^2 |\phi(\mathbf{r}')|^2 (1 - 3 \cos^2 \theta_{\mathbf{e}}) / |\mathbf{r} - \mathbf{r}'|^3$ with $\theta_{\mathbf{e}}$ being the polar angle of $(\mathbf{r} - \mathbf{r}')$. The total Hamiltonian under the SMA is then

$$H_{\text{tot}} = (c'_2 - c'_d) \hat{\mathbf{L}}^2 + 3c'_d (\hat{L}_z^2 + \hat{n}_0). \quad (4)$$

Before we discuss the ground state of H_{tot} , we want to point out that H_{sp} in (1) possesses $\text{SO}(3)$ symmetry, i.e.,

it is rotationally invariant in spin space [20]. The presence of the dipolar interaction, however, breaks this symmetry. This is not unlike the situation in superfluid ^3He , where the dipolar interaction between nuclear spins, despite of its smallness, breaks the spin-orbit symmetry and is crucial for the understanding of the superfluid phases of the system [26]. As we shall see below, the dipolar interaction of atomic spins also results in new quantum phases in spinor condensate.

From Hamiltonian (4), one can expect that the behavior of the dipolar spinor condensate should be very sensitive to the signs of both $(c'_2 - c'_d)$ and c'_d . Unlike c'_2 , both the sign and the magnitude of the dipolar interaction coefficient c'_d depend on the geometric shape of the condensate, which makes the system highly tunable through the modification of the trap aspect ratio. As an example, we assume the condensate wave function has a Gaussian form $\phi(\mathbf{r}) = \pi^{-3/4} \kappa^{1/2} q^{-3/2} e^{-(x^2+y^2+\kappa^2 z^2)/(2q^2)}$, simple calculation shows that [5],

$$c \equiv c'_d / |c_2| = 2\pi c_d \chi(\kappa) / (3|c_2|), \quad (5)$$

where $\chi(\kappa)$ is a monotonically increasing function of the condensate aspect ratio κ , bounded between -1 and 2 , and passing through zero at $\kappa = 1$ [27]. From this it is clear that both the sign and the strength of the effective dipolar interaction can be tuned with trapping geometry.

To gain more insights into the structure of the ground state, let us first neglect the n_0 -term in H_{tot} . The remaining Hamiltonian, denoted by $H_0 [= (c'_2 - c'_d) \hat{\mathbf{L}}^2 + 3c'_d \hat{L}_z^2]$, has a diagonalized form under the basis states $|l, m\rangle$. The ground state of H_0 can be easily found and the phase diagram is illustrated in Fig. 1. We see that the ground state of H_0 is divided into three regimes in the c'_2 - c'_d parameter space, and the ground state angular momentum quantum number l can be either N or 0 .

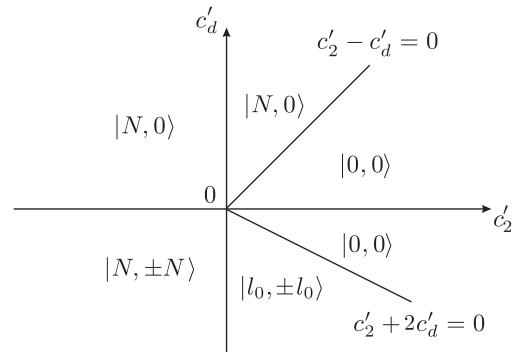


FIG. 1: The ground states of H_0 , where $l_0 = N$ if $N > (c-1)/(2c+1)$, otherwise $l_0 = 0$. For typical parameters, the inequality is usually satisfied, so we can always take $l_0 = N$.

For the case of $l = N$, we expect the ground state of the total Hamiltonian H_{tot} to be very close to that of H_0 , since the n_0 -term is at least a factor of $1/N$ smaller than the rest. In contrast, for the $l = 0$ case, the n_0 -term is expected to be important and the true ground state

should deviate from $|0, 0\rangle$ significantly unless $c = 0$. We found the ground state of H_{tot} numerically by expanding the Hamiltonian onto a Fock state basis $|N_{-1}, N_0, N_1\rangle$ with the constraint $N = \sum_{\alpha} N_{\alpha}$, and the calculations confirmed our qualitative arguments above. In the following, we will discuss the properties of the ground state in more detail and we will present our results for the cases $c'_2 > 0$ and $c'_2 < 0$ separately.

$c'_2 > 0$ case: Figure 2 (a) illustrates the overlap between the true ground state (denoted by $|G\rangle$) and that of H_0 . The overlap is unit in the regions $c < -1/2$ and it quickly approaches unit for $c > 1$. For $-1/2 < c < 1$, the overlap decreases rapidly from 1 when c deviates from 0. In this region, in general $|G\rangle = \sum_l g_l |l, 0\rangle$, with the coefficients g_l dependent upon c , is a superposition of different angular momentum states with $\langle \hat{L}_z \rangle = 0$. The normalized ground state population and its variance are presented in Fig. 2 (b) and (c). Two sharp phase boundaries can be seen at $c = -1/2$ and $c = 1$ in agreement with Fig. 1. The variance is presented in terms of Mandel Q -factor. $Q < 0, = 0$, and > 0 represent sub-Poissonian, Poissonian, and super-Poissonian distributions, respectively. In particular, $Q = -1$ represents a Fock state with vanishing number fluctuations.

For $c < -1/2$, $|G\rangle = |N, \pm N\rangle$ is a Fock state with all the population in either $m_F = 1$ or -1 state. This is the state with spontaneous magnetization discussed in Ref. [25]. Since the ground state in this regime is two-fold degenerated with opposite magnetization, a chain of such condensates will form an example of the Ising model of statistical mechanics. For $c > 1$, $|G\rangle \approx |N, 0\rangle$. Expanded onto the Fock state basis $|N_{-1}, N_0, N_1\rangle$, we have $|N, 0\rangle = \sum_{k=0}^{N/2} g_k |N/2-k, 2k, N/2-k\rangle$ (assuming N to be even), where for $N \gg 1$, the expansion coefficients $g_k = (8/N\pi^2)^{1/4} \exp[-4(k - N/4)^2/N]$, from which we immediately have $\langle \hat{n}_0 \rangle = 2\langle \hat{n}_{\pm 1} \rangle = N/2$, $Q_0 = -1/2$ and $Q_{\pm 1} = -3/4$. Hence the populations in all three spin components have sub-Poissonian distributions. Finally, for $-1/2 < c < 1$, population in $m_F = 0$ state has a super-Poissonian fluctuation with maximum fluctuations occur at $c = 0$, while the population fluctuations in $m_F = \pm 1$ approach the Fock state limit for positive c .

$c'_2 < 0$ case: For this case, the overlap between the true ground state and that of H_0 is nearly perfect. The phase diagram is characterized by a sharp boundary at $c = 0$, and the ground state is given by the maximally polarized state $|N, \pm N\rangle$ or $|N, 0\rangle$ for $c < 0$ and $c > 0$, respectively. Since the phase boundary occurs at $c = 0$ (vanishing dipolar interactions), this phase transition should be readily verifiable in ^{87}Rb spinor condensates by changing the condensate shape from cigar to pancake, or vice versa. As we have mentioned earlier, without the dipolar interaction, the ground state of a ferromagnetic spin-1 condensate is given by $|N, m\rangle$ for any integer m between $-N$ and N (i.e., the spin vector has no preferred spatial orientation). Now the dipolar interaction breaks this degeneracy and orients the spin vector along (perpendicular to) the axial direction for a cigar-shaped (pancake-shaped) con-

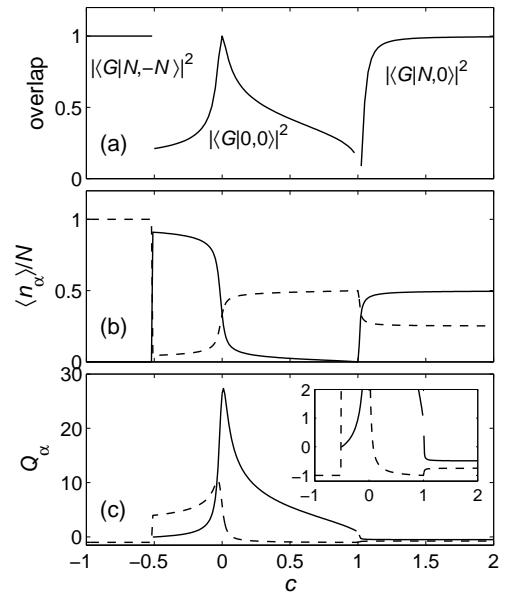


FIG. 2: The c -dependence of the overlap between the true ground state $|G\rangle$ and that of H_0 (a), the normalized ground state population (b), and the number fluctuation (c). The solid and dashed lines in (b) and (c) denote the $m_F = 0$ and -1 components respectively. The inset in (c) shows the detailed behavior of Q_{α} at the vicinity of $Q_{\alpha} = 0$. The results presented here are for $c'_2 > 0$ and $N = 100$ [28].

densate, a clear manifestation of the symmetry-breaking properties of the dipole force.

In addition to the ground state phase structures, the spin-mixing dynamics [21] of the dipolar spinor condensate can also be studied by numerically evolving an initial state under H_{tot} . Figure 3 illustrates one example. Here the initial state is given by the Fock state $|N/2, 0, N/2\rangle$ with half population in $m_F = 1$ and -1 components, respectively. The spin-mixing dynamics will quickly drive the system into a quasi-steady state. Again we want to focus on the effect of the dipolar interactions whose strength depends on the condensate aspect ratio κ . In Fig. 3 the steady state population of spin-0 is plotted as a function of c , while the inset replots the population as a function of κ using parameters for ^{87}Rb . As we can see, modifying the condensate aspect ratio changes significantly the population distribution in the steady state.

In summary, we have studied the ground state properties and spin-mixing dynamics of a dipolar spinor condensate. We have shown that the dipolar interaction breaks the rotational symmetry of the Hamiltonian and as a result the ground state is characterized by several distinct quantum phases depending on the relative strengths of the spin-exchange and dipolar interactions. The transitions between these phases may be induced by simply modifying the trapping geometry of the condensate.

We have neglected any external magnetic field in our study here. The presence of external fields will affect the orientation of the spin and hence change the phase di-

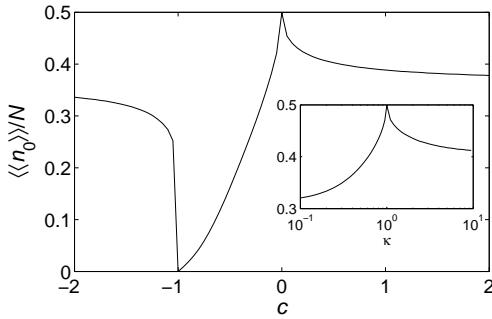


FIG. 3: The c -dependence of the steady state population of $m_F = 0$ component for the initial state $|N/2, 0, N/2\rangle$ with $N = 10^4$ and $c'_2 < 0$. The inset indicates its κ -dependence for ^{87}Rb condensate with a Gaussian wave function.

agram. For the change to be insignificant, we need to reduce the field strength such that the zeeman energy is weaker than the dipolar energy. For typical values of alkali atoms, this requires to control the magnetic field below 10^{-4} Gauss [29]. This requirement will pose an experimental challenge (none of the experiments on spinor BEC so far [16, 17, 18, 19] has met this field-free requirement), but is within reach with current technologies. We hope our work will stimulate experimental efforts along this line. The effect of the magnetic field on dipolar spinor condensates is currently under study. Our future works will also include the study of spin-2 dipolar spinor condensate [18, 19]. We believe that these studies will open many unexplored and promising avenues of research in the field of quantum degenerate atomic gases.

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[27] The choice of the Gaussian ansatz is a matter of convenience. Essentially the same results are obtained for a parabolic ansatz (C. Eberlein, S. Giovanazzi, D. H. J. O'Dell, cond-mat/0311100). In general, $c'_d < 0$ ($c'_d > 0$) for a cigar-shaped (pancake-shaped) condensate.
[28] Obviously the maximum total number of atoms used in the calculations are limited by computer power. However, we have found essentially the same behavior for N from a few tens to around 100. So we believe the results are valid for realistic atomic numbers ($10^4 \sim 10^6$).
[29] This requirement can be relaxed a little if atoms with larger magnetic moment (e.g., Cr, Sr, etc.) can be used. But none of these atoms has been condensed so far.